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Large-eddy simulation of a backward facing step flow using a least-squares spectral element method

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We report preliminary results obtained from the large eddy simulation of a backward facing step at a Reynolds number of 5100. The numerical platform is based on a high order Legendre spectral element spatial discretization and a least squares time integration scheme. A non-reflective outflow boundary condition is in place to minimize the effect of downstream influence. Smagorinsky model with Van Driest near wall damping is used for sub-grid scale modeling. Comparisons of mean velocity profiles and wall pressure show good agreement with benchmark data. More studies are needed to evaluate the sensitivity of this method on numerical parameters before it is applied to complex engineering problems.

1. Introduction

Many aerospace and commercial products operate in a dynamic flow environment. The structural integrity, performance, and development costs of these products are affected by the unsteady flowfields they encounter. In rocket propulsion systems, dynamic loads are the cause of many life limiting and failure mechanisms. For instance, a number of dynamic load related issues manifested themselves during the development of the space shuttle main engine, resulting in hundreds of millions of dollars of program development costs in terms of hardware redesign and testing. Unsteady flows can also be a very effective sound generating mechanism; George (1990) states that the aerodynamically generated noise increases approximately as velocity to the 6th power. Therefore, the aerodynamic noise generated by vehicles traveling at high speeds can be very annoying to both passengers and communities located in the proximity of major highways and railroads. In some European countries where trains can travel in excess of 200 MPH, the responsible agency has to erect sound walls along the railroads to minimize the effects of noise pollution. This requirement can drastically increase the construction and maintenance costs of a railway system. For passenger cars, unacceptable noise levels inside the compartment can have adverse effects on sales.

In light of the importance in characterizing the dynamic flow environment in both aerospace and commercial applications, Rocketdyne has initiated a multi-year effort to develop a general purpose computational fluid dynamics based analysis system for dynamic load prediction. This system will provide high-fidelity predictive capability through the development of a novel numerical algorithm and

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utilization of distributed parallel computing. The numerical algorithm is a high order spectral method which provides the unique capability to accurately model complex geometries and rapidly varying flowfields. Parallel computing provides the necessary memory capacity and speed required for large scale computations. All these features have been incorporated in the Rocketdyne Unstructured Implicit Flow (UniFlo) solver. The UniFlo code is capable of performing a hierarchy of fluid dynamic analyses including direct numerical simulation (DNS), large eddy simulation (LES) and Reynolds average Navier-Stokes solution (RANS). Only DNS and LES can provide time accurate information that is needed for unsteady turbulent simulations. LES models flow features that are not directly captured by the grid resolution employed. This technique is also known as subgrid scale (SGS) modeling. The LES approach (vs. DNS) can relax the requirement on grid resolution that is normally very demanding for turbulent flow simulations making it an effective tool for engineering analyses. However, one also has to be concerned with the numerical errors that increase as the grid is coarsened. If not controlled properly, these errors can overwhelm the advantage offered by LES. Therefore, the purpose of this work is to first evaluate the numerical accuracy of UniFlo in predicting time dependent flows. Once this is accomplished, we then assess the capability of the Smagorinsky SGS model in predicting turbulent flow. The backward facing step configuration is chosen as the benchmark case since it mimics the flowfield in a rocket engine combustor and existing numerical and experimental data are available for comparison.

In what follows, we describe the numerical method, boundary condition and SGS model employed by UniFlo. Numerical results demonstrating accuracy of the method and effectiveness of the Smagorinsky model are also provided.

2. Numerical method

The Navier-Stokes equations are written as a first order system and can be represented as $\mathcal{L}\vec{u} = \vec{f}$ in a domain $\Omega \subset \mathbb{R}^{n_d}$ which is subjected to the condition $B\vec{u} = \vec{g}$ along a piecewise smooth boundary Γ . \mathcal{L} is a first-order partial differential operator:

$$\mathcal{L}\vec{u} = \sum_{i=1}^{n_d} \mathcal{A}_i \frac{\partial \vec{u}}{\partial x_i} + \mathcal{A}_0 \vec{u}$$

$n_d = 2$ or 3 , depending on the spatial dimensions, x_i 's are the Cartesian coordinates, \vec{u} has a length n , where n is the number of dependent variables, \vec{f} is the forcing function, and both B and \vec{g} describe the appropriate boundary conditions. \mathcal{A} 's are $m \times n$ matrices which describe the characteristics of the system of equations being solved. The idea behind the least squares spectral element method (LSSEM) is to minimize the residual

$$R = \mathcal{L}\vec{u} - \vec{f}$$

in a least squares sense within the domain of interest and construct the functional as

$$I(\vec{u}) = \frac{1}{2} \|\mathcal{L}\vec{u} - \vec{f}\|_0^2 = (\mathcal{L}\vec{u} - \vec{f}, \mathcal{L}\vec{u} - \vec{f})$$

By setting $\delta I = 0$ and $\delta \vec{u} = \vec{w}$, one can reduce the problem to

$$(\mathcal{L}\vec{w}, \mathcal{L}\vec{u}) = (\mathcal{L}\vec{w}, \mathcal{L}\vec{f}) \quad \vec{w} \in S$$

where, $S = \{\vec{u} \in H_0^1(\Omega); B\vec{u} = g \text{ on } \Gamma\}$, and H_0^1 is the Sobolev space with a compact support. For incompressible viscous flows, the working variables are velocity, pressure, and vorticity. By using this system of equations, one can employ any of the C^0 functions to approximate the spatial variation of the dependent variables. UniFlo employs isoparametric mapping to transform the governing equations from the Cartesian coordinate system to a generalized coordinate system where the spatial discretization is performed. The domain of interest is divided into a set of non-overlapping elements and within each element, basis function derived from Legendre polynomials is used for spatial discretization. The spatial accuracy depends on the choice of the order of Legendre polynomial basis function and can vary from element to element. This approach, also known as spectral element, has been formulated by Rønquist and Patera (1987). LSSEM uses a common interpolating function to approximate all of the dependent variables. Even with the presence of the convective terms, the resulting set of algebraic equations are positive definite and symmetric. LSSEM maintains a tight coupling among all of the governing equations and provides a set of well-defined boundary conditions that are consistent with flow physics and mathematical constraints. It does not require any user defined artificial damping factor to maintain numerical stability. To maintain high spatial accuracy at the domain boundary, UniFlo does not need special treatment such as the utilization of ghost points. The convective terms are linearized with the Newton-Raphson procedure so that the spatial derivatives can be discretized implicitly. Sub-iterations are required at each time step for the purpose of minimizing the effect of linearization errors. For most problems, the residual can be reduced by four orders of magnitude in less than three iterations. The accuracy is second order in time with the application of a backward differencing scheme. For instance, the temporal derivative of the velocity component, u , can be discretized as

$$\frac{\partial u}{\partial t} = \frac{u^{s-1} - 4u^s + 3u^{s+1}}{2\delta t}$$

where superscripts represent different time levels. The resulting algebraic equations are solved by the conjugate gradient method with Jacobi preconditioning. The structure of the coefficient matrix is completely arbitrary and the solution procedure does not rely on any pre-defined order. More details of this method is given by Chan (1996).

The boundary conditions are: (1) specified velocity at the inlet, (2) no slip along solid walls, (3) stress free and vanishing normal velocity component along the plane of symmetry and (4) 'free boundary' along an outflow plane. For a Cartesian grid, stress free condition is imposed by setting the horizontal vorticity components to zero. Points located on a 'free boundary' are treated as unknowns and solved directly.

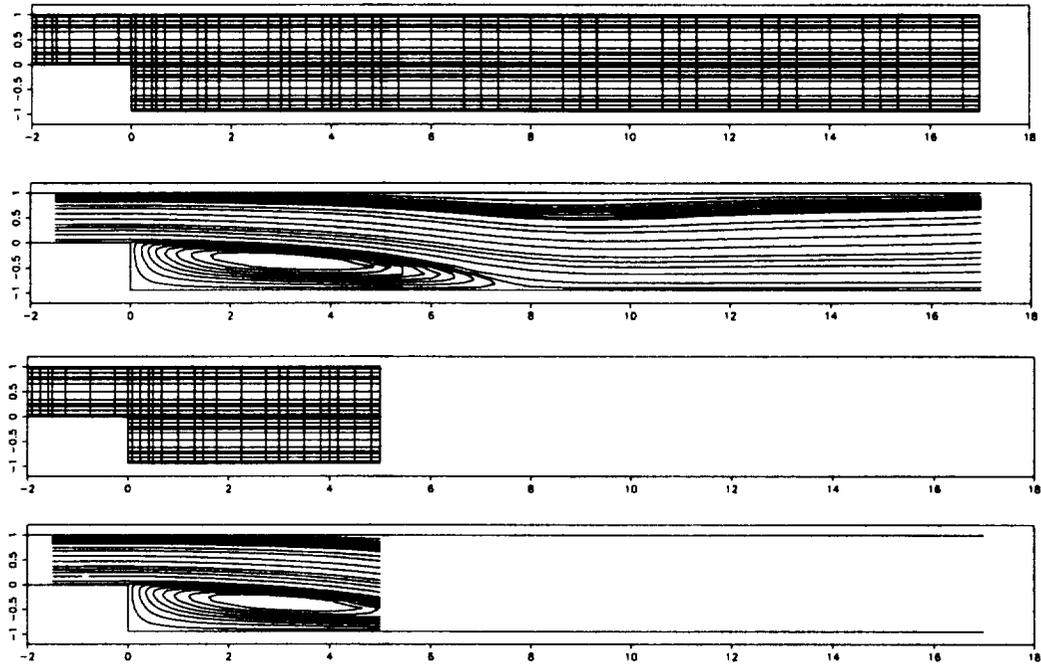


FIGURE 1. Streamlines behind a backward facing step at $Re = 389$; top half: result for long domain; bottom half: result for truncated domain.

For turbulent flows, we relate the subgrid scale stresses to the strain rate of the resolved velocity field via Boussinesq approximation. The diffusion term of the Navier-Stokes equations then becomes

$$-\left(\frac{1}{Re} + \nu_t\right)e_{ijk} \frac{\partial \omega_k}{\partial x_j} - \frac{\partial \nu_t}{\partial x_j} 2S_{ij}$$

where ν_t is the eddy viscosity, S_{ij} is the strain rate, and ω is the vorticity. The value of e_{ijk} is equal to zero unless each of the number 1, 2, and 3 occurs as a subscript. Furthermore, e_{ijk} is equal to 1 if the order of subscripts is cyclic, it becomes -1 if the order of subscripts is not cyclic. The eddy viscosity is computed as

$$\nu_t = (C_s \Delta)^2 |S_{ij}| f_s$$

$$\Delta = (\delta x \delta y \delta z)^{1/3}$$

where $C_s = 0.1$ and f_s is the Van Driest damping function defined as

$$f_s = 1.0 - \exp\left(\frac{-\delta^+}{26}\right)$$

In reality the value of C_s is not constant and can change in time and space. Near a corner, δ^+ is determined with the shortest normal distance from the adjacent walls. This procedure is somewhat *ad hoc* and is problem dependent.

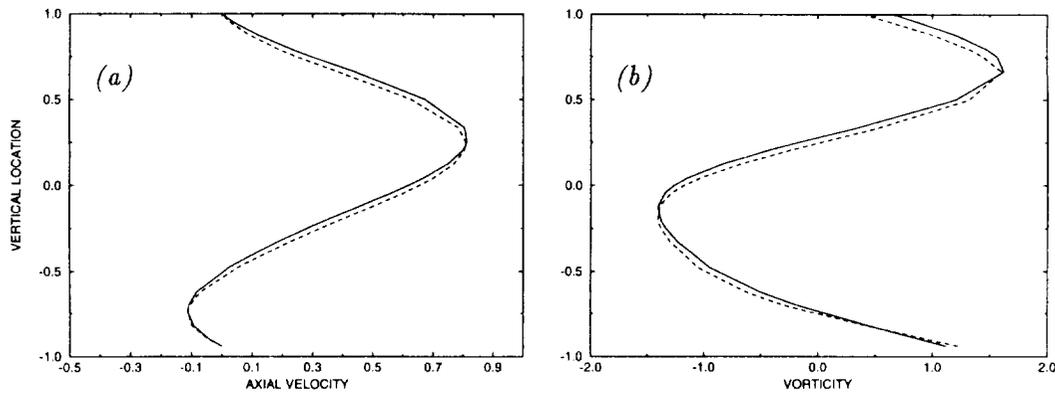


FIGURE 2. Predicted profiles at an axial distance of 5 inlet heights behind a backward-facing step with $Re = 389$, — results obtained with long domain --- results obtained with truncated domain, (a) axial velocity profile and (b) vorticity profile.

3. Numerical results and discussion

To demonstrate the effectiveness of the current outflow boundary condition, we apply it to compute the laminar flow behind a backward facing step studied experimentally by Armaly *et al.* (1983). The Reynolds number, based on the inlet height and average velocity, is 389. The ratio between the inlet and step heights is 0.94. Flow separates behind the step and reattaches at an axial distance that is equal to about eight step heights from the plane of expansion. Two exit domains, one long and one short, are used. For the long domain case, the axial length behind the step is 17, the flow has room to reattach after separation and recover to a fully-developed flow; therefore, the downstream influence on the flowfield near the step is small, and for comparison we can use the predicted profiles as the baseline. For the short domain case, the outflow plane, which cuts through the separated region, is located at 5 inlet heights behind the step. Because of this, accuracy of the predicted profiles is strongly influenced by the outflow boundary condition. For time dependent turbulent flow, this situation is similar to having an eddy pass across an outflow boundary. A parabolic profile is imposed along the inlet plane which is located at 2 inlet heights upstream of the expansion. Figure 1 shows the grid systems and streamlines predicted by UniFlo for both the short and long domains. In both cases, 5 collocation points are placed within each element. The total number of elements is 72 for the long domain and 36 for the short domain. The flow pattern is almost the same in both cases. For the short domain case, having a reverse flow on part of the outflow boundary does not present numerical convergence problem, and this further demonstrates the robustness of the current numerical method and outflow boundary condition. The predicted reattachment is 8.0 times the inlet height and is in good agreement with the test data. Armaly *et al.* also reports that at $Re = 389$, the flow begins to separate from the upper wall and becomes three-dimensional, but the separation region is so small that its size

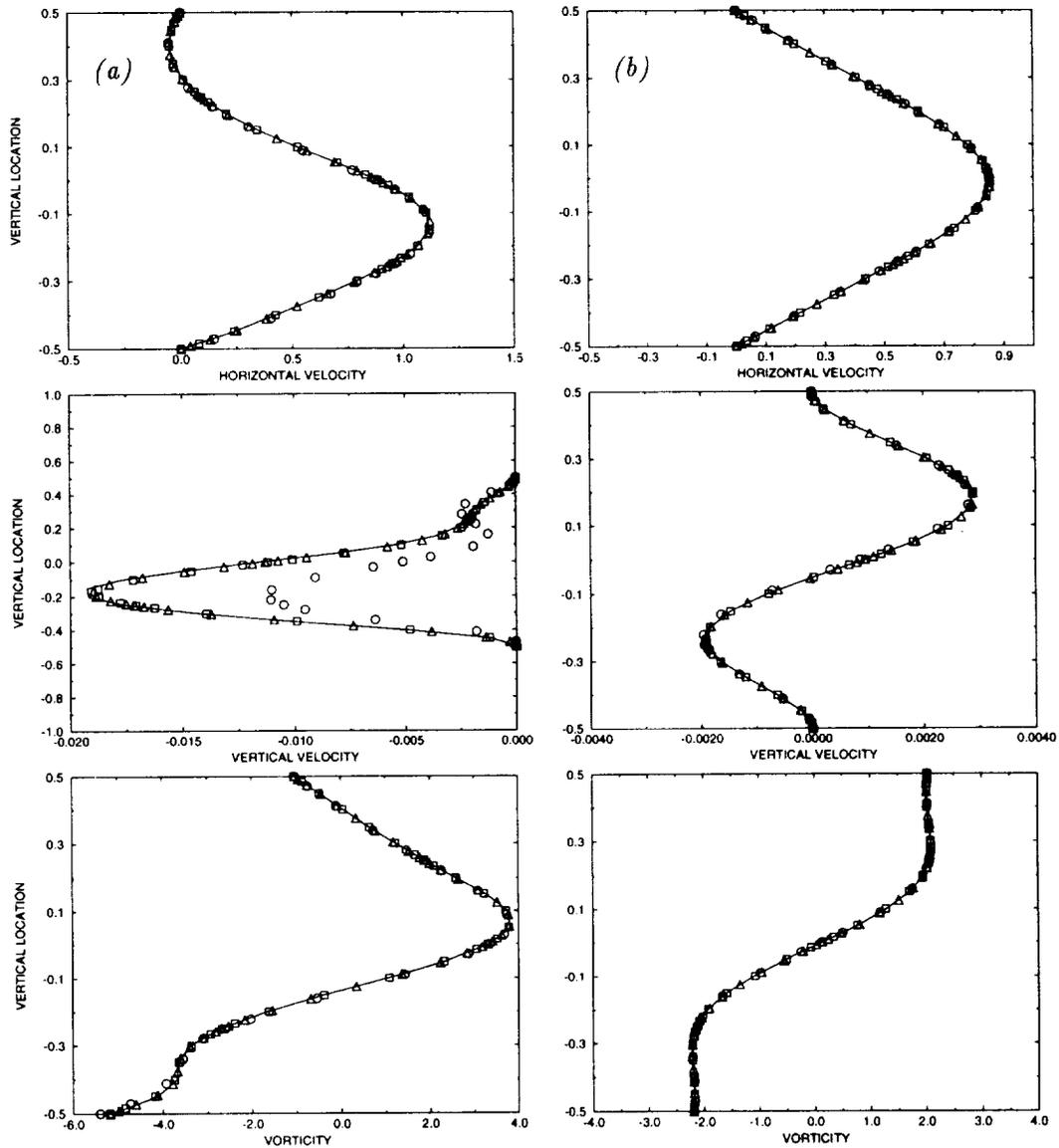


FIGURE 3. Predicted profiles behind a backward-facing step with $Re = 800$; — Gartling's results, \circ 5th order, \triangle 6th order, and \square 7th order; (a) axial location of 7 and (b) axial location of 15.

could not be measured. This phenomena is correctly predicted by UniFlo. Figure 2 shows the axial velocity and vorticity profiles at an axial location of 5 inlet heights behind the step. The trend in both cases is identical, with only less than 10 percent discrepancy on the magnitude.

The next test case is due to Gartling (1990) and Gresho *et al.* (1993). The purpose of this exercise is to answer some of the questions raised by Gresho *et al.* as

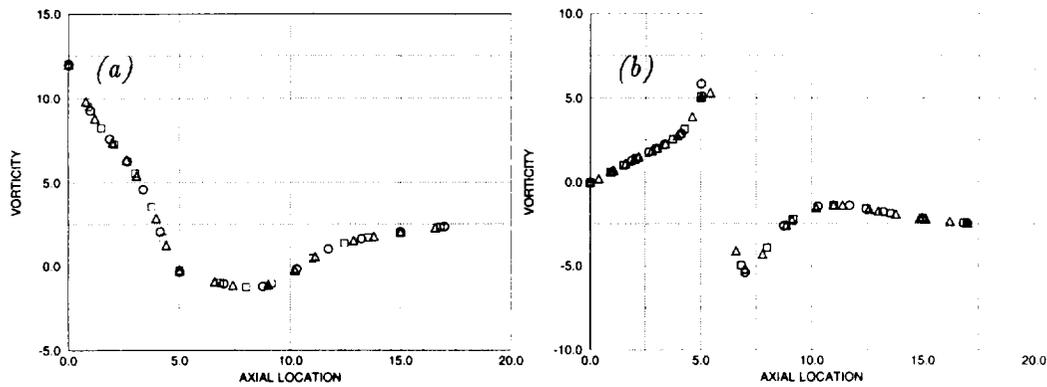


FIGURE 4. Predicted wall vorticity distribution for a backward-facing step with $Re = 800$, \circ 5th order, \triangle 6th order, and \square 7th order, (a) upper wall and (b) lower wall.

to whether spectral methods can handle flow geometries with a sharp corner and predict the correct flow behavior. Through careful numerical studies and stability analysis, they conclude that at a Reynolds number of 800, the flow behind a backward facing step with 1:2 expansion ratio is indeed steady. With this in mind, we first perform the simulation as a steady state problem by turning off the transient terms in the Navier-Stokes equations. The rectangular flow domain is 17 units long and 1 unit high. The flow enters the domain along the top half portion of the left boundary with a parabolic profile. The Reynolds number based on the step height and mean velocity is 800. Figure 4 shows the grid skeleton employed; there are 4 elements in the vertical direction and 11 elements in the streamwise direction. Within each element, we apply 5th, 6th, and 7th order polynomials, respectively, in each of the two directions. Figure 3 shows the comparison between the predicted profiles and benchmark data at two different streamwise locations. All except the vertical velocity profile at the axial location of 7 show an excellent agreement with the benchmark data of Gartling. Figure 4 shows the vorticity distribution, which is proportional to shear stress, along the bottom and top boundaries. By examining these plots, one can determine both the separation and reattachment points. Along the lower wall, UniFlo predicts a reattachment length of 6.1, whereas along the upper wall, it predicts a separation at the streamwise location of 4.8 and a reattachment at the streamwise location of 10.5. These predictions are in excellent agreement with the benchmark data. These results also indicate that for steady flow computation, numerical error incurred from using an under-resolving grid is very localized.

We then compute the same problem by treating it as an unsteady flow. Initially, the flow is stagnant inside the domain. Figure 5 shows the temporal evolution of the streamlines for the case where 6th order polynomials are used inside each element. Overall this grid resolution produces satisfactory results for steady state calculation, however, this is not the case for time accurate simulation. A transient process, which involves a sequence of vortex shedding, takes place along the upper

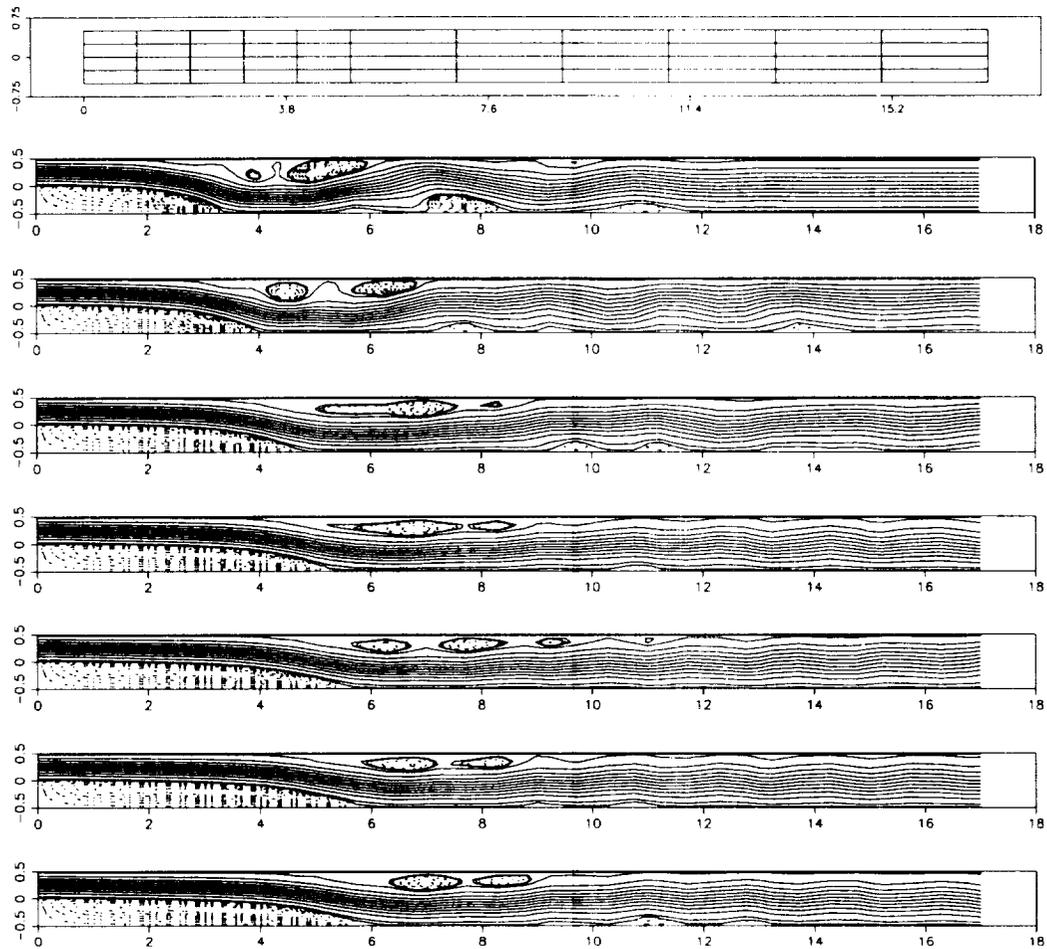


FIGURE 5. Streamlines showing the time evolution of the flowfield behind a backward facing step at a Reynolds number of 800; computation performed with a 11×4 grid and 6^{th} order Legendre polynomials; final state is a temporally periodic flow; from top to bottom: time=10, 20, 30, 50, 80, 100, and 140.

wall at the streamwise location where the steady state result show a discrepancy in the vertical velocity profile prediction. This result demonstrates that numerical error that develops in a small region can grow over time and contaminate the entire flowfield. We then refine the grid by increasing the number of elements in the streamwise direction to 18 while maintaining 6^{th} order polynomials in each element. The result shown in Fig. 6 indicates that the initial transient flow features decay rapidly in time and the flow evolves asymptotically towards a steady state. This prediction agrees with the finding of Gresho *et al.* It is apparent that the transient flow predicted above is a numerical artifact. Unfortunately, the flow features generated by this numerical error look so real, making them difficult to detect. Therefore, for unsteady flow simulation one must perform grid dependence study

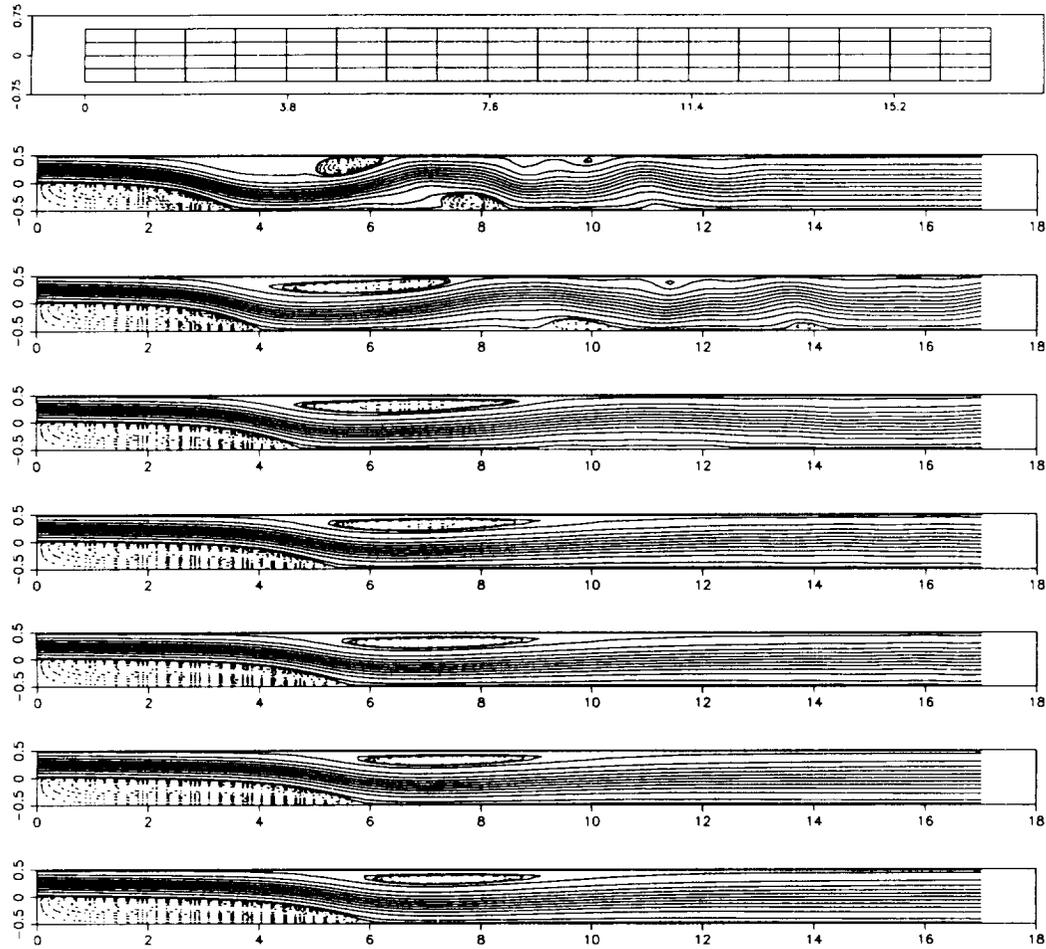


FIGURE 6. Streamlines showing the time evolution of the flowfield behind a backward facing step at a Reynolds number of 800; computation performed with a 18×4 grid and 6^{th} order Legendre polynomials; asymptotic state is steady; from top to bottom: time=10, 20, 30, 50, 80, 100, and 140.

before attempting to explain the underlying flow physics.

Having addressed some of the relevant numerical issues, we then use UniFlo to simulate the three-dimensional backward-facing step configuration where experimental data of Jovic and Driver (1994), DNS data of Le and Moin (1994), and LES data of Akselvoll and Moin (1995) are available for comparison. The grid system employed is shown in Fig. 7. There are 13 elements in the streamwise direction, 6 elements in the vertical direction and 6 elements in the spanwise direction. Within each element, 6^{th} order Legendre polynomials are used in each of the three directions. The expansion ratio is 5:6. The geometry is scaled with the step height, H . The inlet plane is located at $5H$ upstream of the expansion, and the outflow plane is located at $17H$ downstream of the expansion plane. The spanwise width is $4H$ and

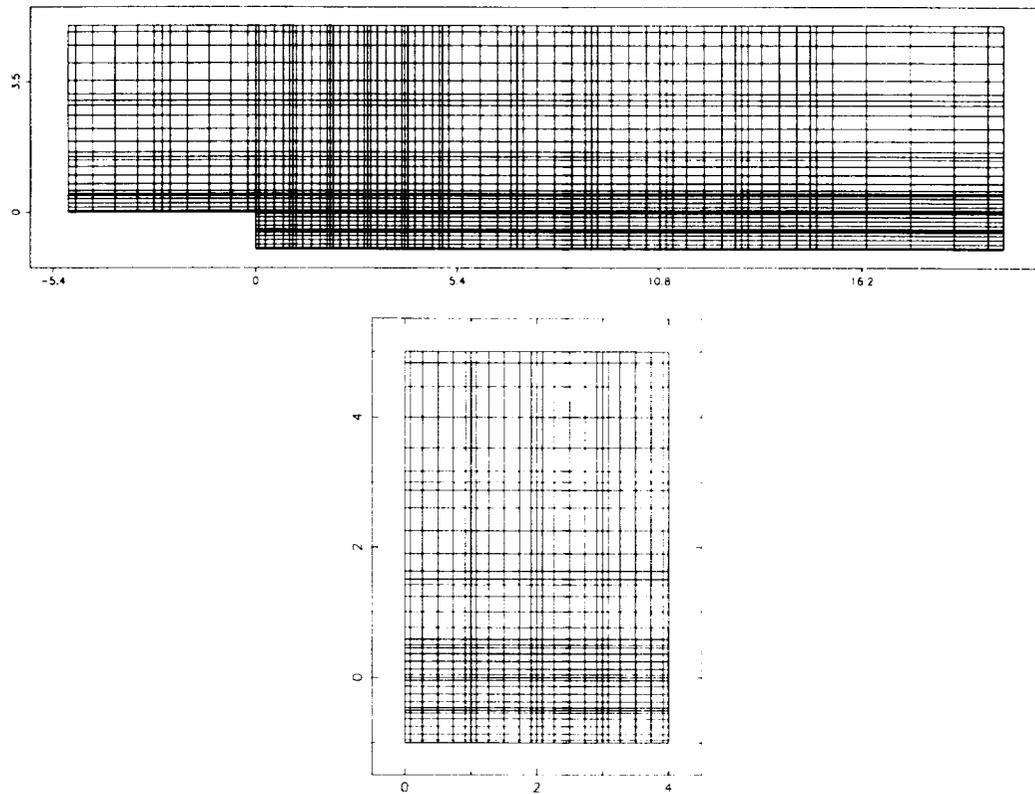


FIGURE 7. Grid system for the three-dimensional backward facing step, top: through flow plane, bottom: cross-sectional plane.

a periodic boundary condition is imposed in this direction. Stress free condition is imposed along the top boundary, and no slip condition is imposed along the bottom wall. At the inlet plane, we take the time dependent turbulent boundary layer profiles computed by Akselvoll and Moin and interpolate them onto the current grid. The freestream velocity is taken to be one, and the time it takes for the flow to travel one step height is also one. Since our implicit flow solver is not restricted by the CFL condition for numerical stability, we can take a larger time step size of 0.1, which is five times higher than that employed by Akselvoll and Moin. As a result, each through flow takes 220 time steps. Time average quantities are collected after the flow has evolved through the domain 5 times. For comparison, we further average the data in the spanwise direction and show them in Fig. 8. The predicted wall pressure distribution is in good agreement with the experimental data inside the recirculating region behind the step. However, in the recovery region, all the numerical methods, including UniFlo, predict a faster recovery rate than that of the experimental measurements. The velocity profiles are compared to the DNS data of Le and Moin. The agreement is good for all five streamwise locations.

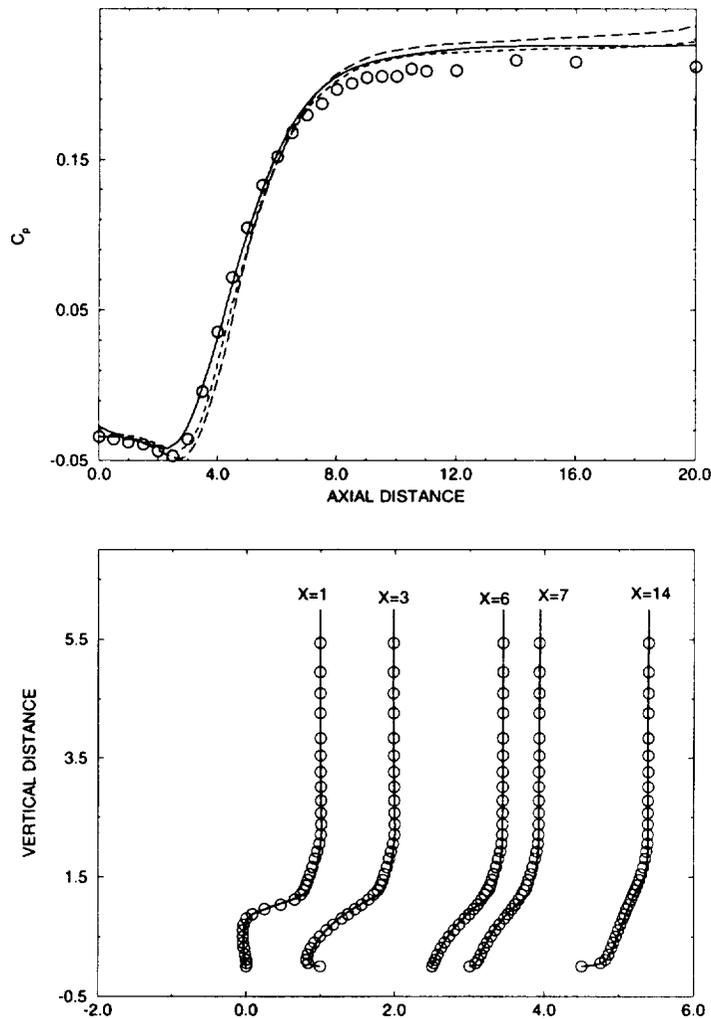


FIGURE 8. Time and spanwise average flow quantities predicted by UniFlo for a three-dimensional backward facing step at $Re = 5100$, top: pressure coefficient along bottom wall, — UniFlo prediction, --- DNS result of Le & Moin ---- LES result of Akselvoll & Moin, and \circ experimental result of Jovic & Driver; bottom: axial velocity profiles at selected streamwise locations; — UniFlo, \circ DNS result of Le & Moin.

4. Summary

We have demonstrated that a spectral based flow solver can be used to simulate the flow behind a backward-facing configuration. The weak singularity located at the corner does not present numerical problem to the least squares method. Numerical error can generate unsteady flow phenomena that could be mistaken as 'real' flow physics. Therefore, grid dependence study is paramount (more so than

the steady state flow calculation) in unsteady flow simulation. The preliminary results obtained from the LES show good agreement with both experimental data and numerical data. Further studies are needed in order to understand the role of the subgrid scale model in these simulations. The Smagorinsky model with Van Driest wall damping is, however, difficult to implement for complex geometries. Future work will include the implementation of dynamic models that do not require wall damping function and user specified model constant.

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